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Kinetic Monte Carlo simulations of void growth in metals under irradiation¹ G.S. BALES, J. BELAK, J.E. KLEPEIS, Lawrence Livermore National Laboratory, Livermore, CA 94551 — The nucleation and growth of voids and interstitial clusters in metals under irradiation is studied with kinetic Monte Carlo (KMC) simulations and self-consistent mean field rate equations. Special emphasis is placed on the effect of the microstructure (grain boundaries, etc) on the void growth and swelling rate. Direct comparison of the numerical solution to the rate equations and the KMC simulations reveals the importance of a self-consistent approximation to the rate coefficients which includes the correct topology of the microstructure. For example, diffusion of point defects along and the nucleation of voids on the grain boundaries is computed with the correct two-dimensional form for the capture numbers which are coupled self-consistently to diffusion and nucleation in the bulk. The mobility of individual point defects (vacancies and interstitials) and small clusters are estimated with molecular dynamics simulations and first principles calculations.

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